

3-Deoxy-manno-oct-2-ulopyranosonic acid
10149-14-1 | DTXSID80143949

Model Performance

Model	Data
-------	------

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 313 °C

Global applicability domain: Outside

Local applicability domain index: 8.97e-02

Confidence level: 5.57e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Erythritol</div> <div>Measured: 331</div> <div>Predicted: 327</div>	<div>Image not found</div> <div>Pyrogallol</div> <div>Measured: 309</div> <div>Predicted: 292</div>	<div>Image not found</div> <div>Triisopropanolamine</div> <div>Measured: 305</div> <div>Predicted: 302</div>
<div>Image not found</div> <div>Triethanolamine</div> <div>Measured: 335</div> <div>Predicted: 326</div>	<div>Image not found</div> <div>2-(Hydroxymethyl)-2-methyl-1,3-propanediol</div> <div>Measured: 283</div> <div>Predicted: 289</div>	